magnetic field defects the ions
Electric field accelerates the ions
Path of heavier ion
Vacuum pump
Electrons ionise the sample
Vaporised sample
Path of lighter ion
detector

Spectra of monatomic Elements

mass spectrum of Boron
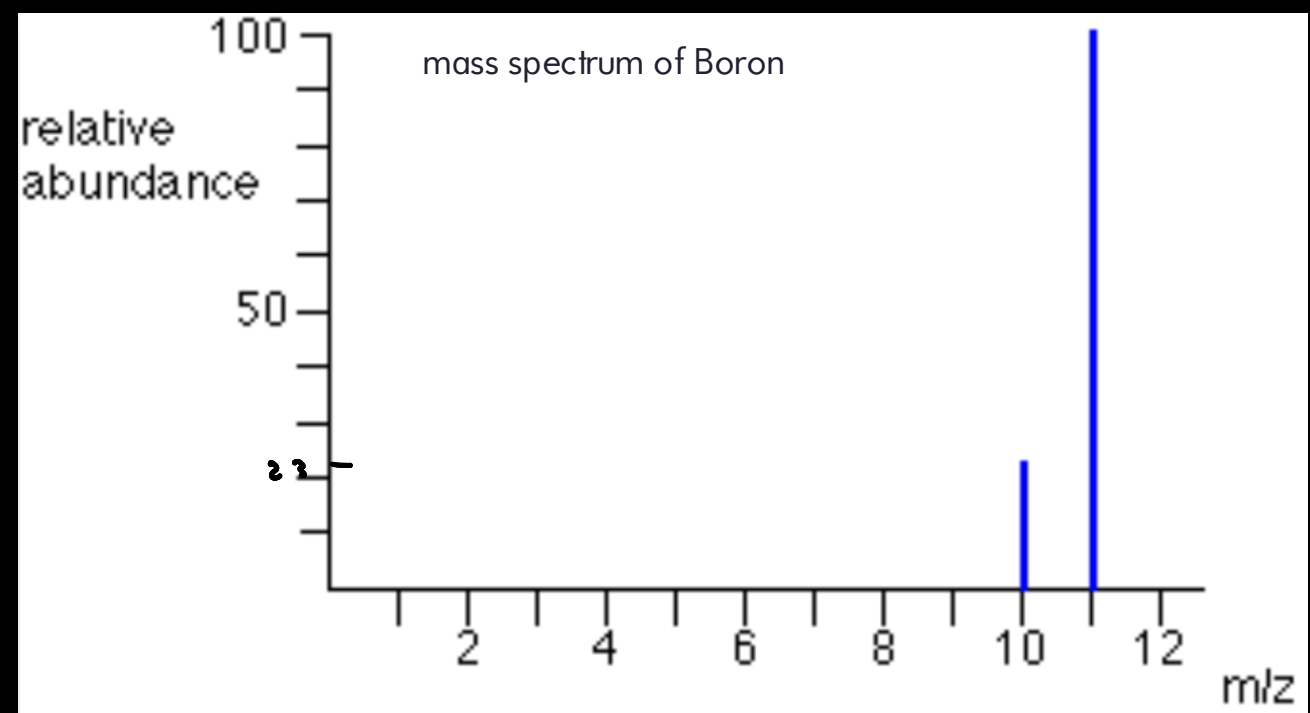
R.A.M = Σ (isotope mass × isotope abundance) / 100
For this example the abundance for :
B-10 is $\frac{22}{123} \times 100\% = 18.7\%$
B-11 is $\frac{100}{123} \times 100\% = 81.3\%$

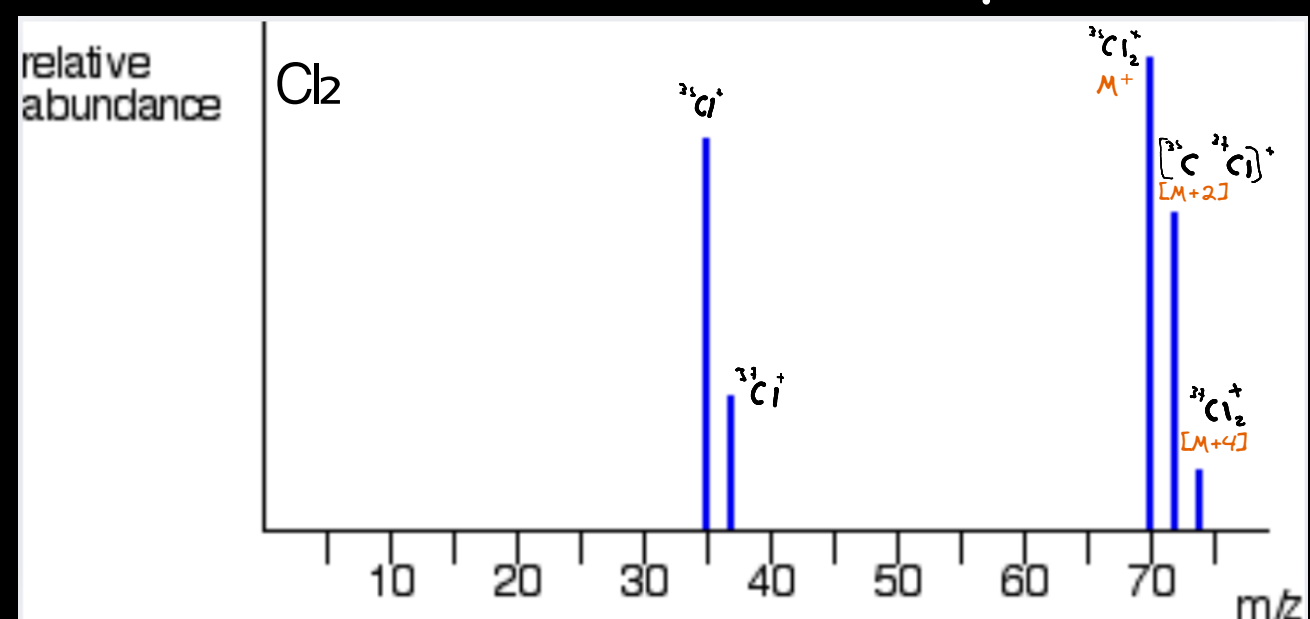$R.A.M = \frac{(10 \times 18.7) + (11 \times 81.3)}{100} = 10.8$

Note:
Sometimes two electrons are removed forming a 2+ charged ions.
Ex   Species : $^{10}B^{2+}$ $m/z = \frac{10}{2} = 5$
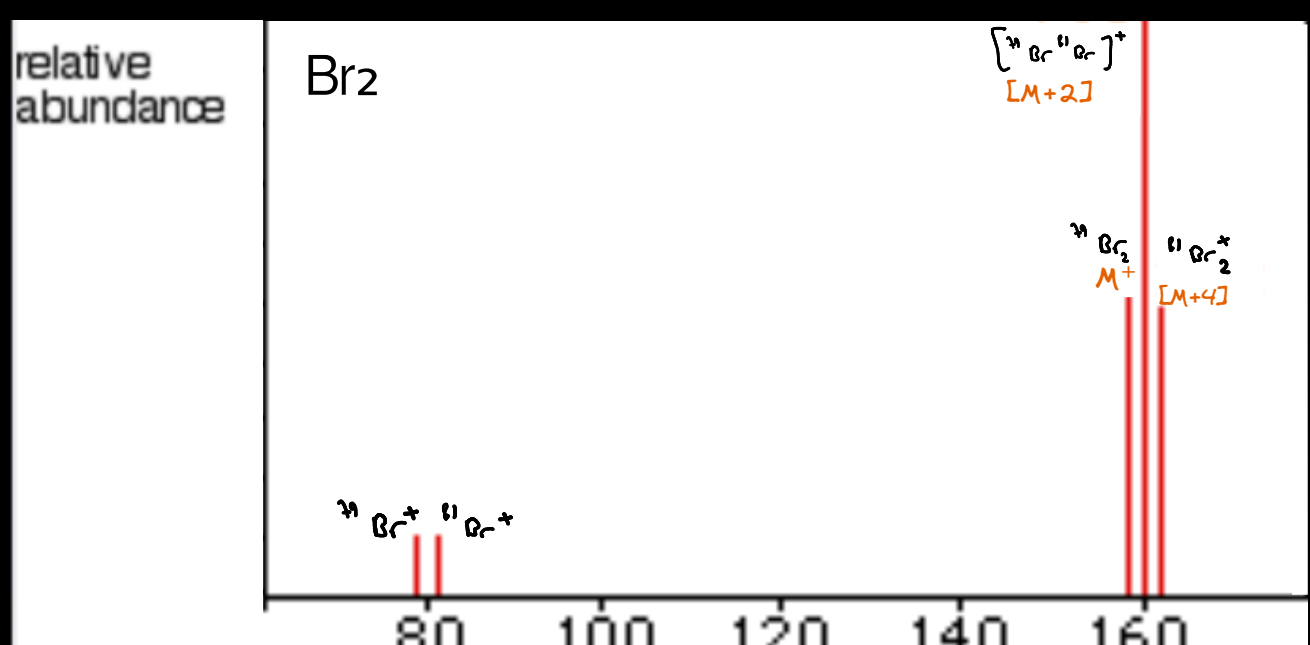
Stages of Mass Spectrometry

Vaporization: The sample must be in its gaseous state so that its particles can move through the machine.

Ionization: High-energy electrons collide /bombard the sample, knocking out one or more electrons (mostly only 1) from the atoms or molecules, thereby creating positive ions.

Acceleration: The ions are accelerated by an electric field. They then pass through a velocity selector, which ensures all ions are moving at the same velocity(won't be responsible for difference in deflection).

Deflection: The ions are deflected by a magnetic field. The amount of deflection depends on the mass-to-charge ratio (m/z) of the ions.

Detection: The deflected ions pass through a narrow slit and collected on a metallic plate connected to an amplifier. The detector detects how many ions pass through the machine. It shows how many ion have this mass-to-charge ratio(m/z).

----->Only ions with a specific mass-to-charge ratio will be deflected precisely enough to pass through the slit for a given magnetic field strength.
(Larger m/z results in a lower delfection and vise versa)

----->The magnetic field strength is varied steadily to detect ions with different mass-to-charge ratios.

Why is there a vacuum in the spectrometer ?
1- Ions might collid in air deflecting them from their normal path
2-Air particles can cause additional/false peaks

mass spectrum of pentan-2-one - CH3COCH2CH2CH3
43
71
86 M+
87 M+1
this M+1 peaks is caused by C-13 (it has a low percentage off being present thats why it has a lower peak)

When a molecule or compound is ionized using high-energy electrons not only does it lose an electron (froming a Molecular/parent ion (M+) which is the Mr of compound) it gets fragmented leading to a number of peaks corresponding to fragments formed)

Spectra of Molecules
Chlorine

relative abundance   Cl2
$^{35}Cl^+$
$^{37}Cl^+$
$^{35}Cl_2^+$ M+
$[^{35}C \, ^{37}Cl]^+$ [M+2]
$^{37}Cl_2$ [M+4]

---the ratio of the peak heights for Chlorine atoms is 3:1 (as the relative abundance of Cl-35 is 3x greater than that of Cl-37)
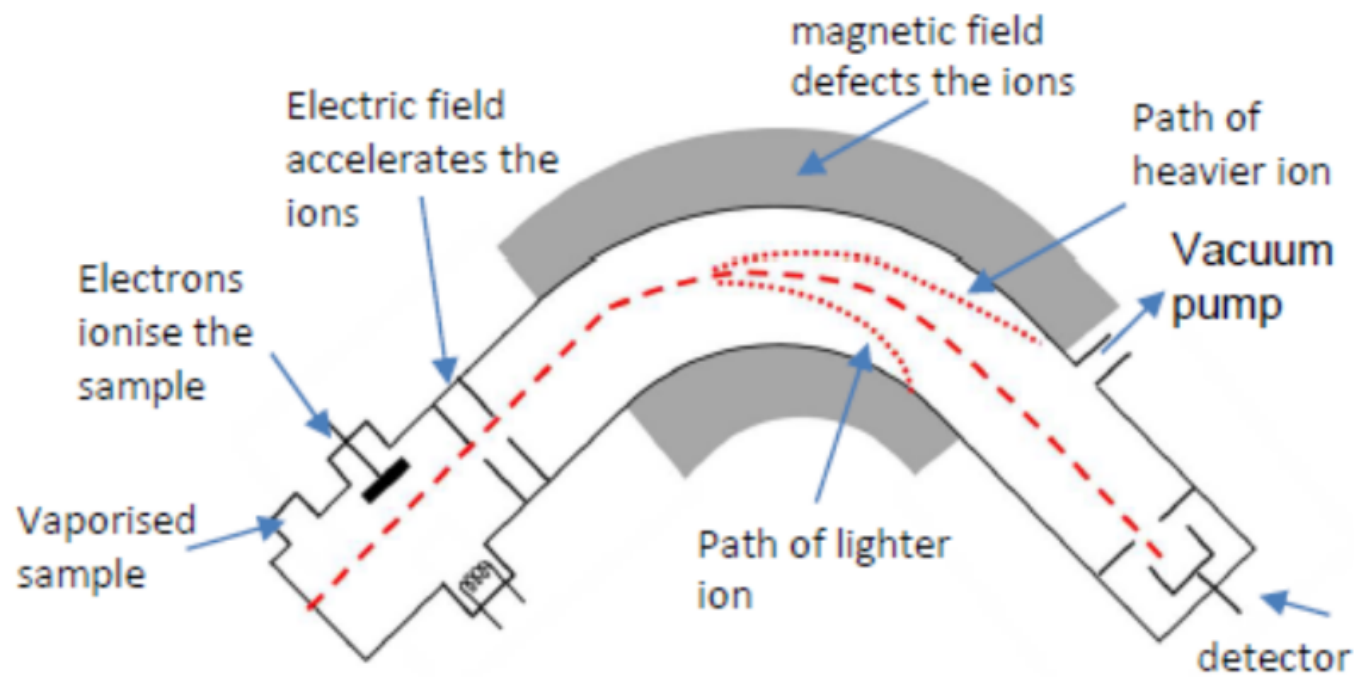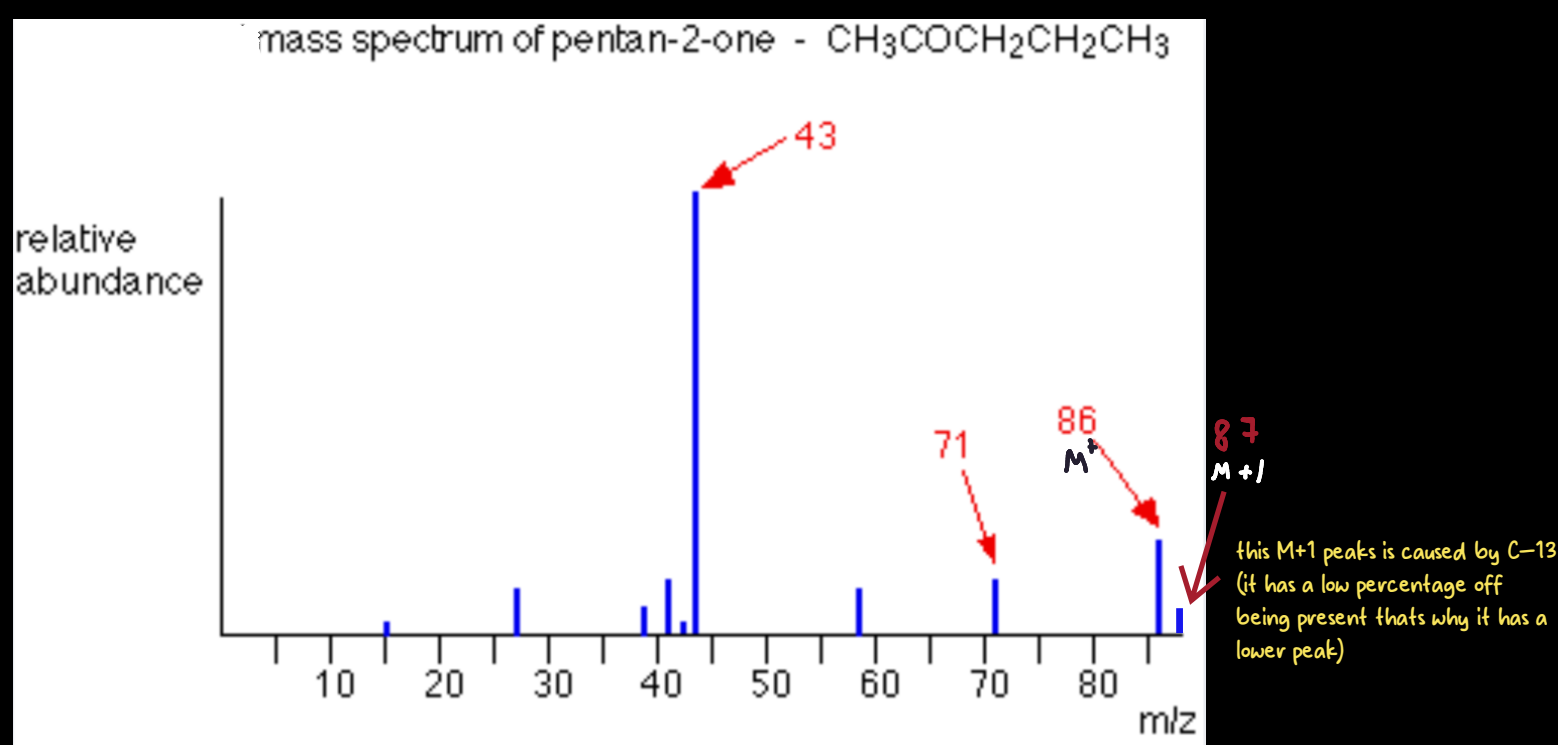---the ratio of the peak heights for Chlorine molecules is 9:4:1

Bromine

relative abundance   Br2
$[^{79}Br \, ^{81}Br]^+$ [M+2]
$^{79}Br_2^+$ M+
$^{81}Br_2^+$ [M+4]
$^{79}Br^+$ $^{81}Br^+$

---the ratio of the peak heights for Bromine atoms is 1:1 (as the relative abundance of Cl-79 is the same as that of Cl-81)
---the ratio of the peak heights for Bromine molecules is 1:2:1

Your Notes

Quantum mechanics

Each principal quantum shell is split into subshells (s,p,d and f) and each it split into samller regions called orbitals (each orbital holds a max. of 2 electron only)

The electrons fill the subshells starting with the one with least energy(1s) and going up the energy(s < p < d < f)

Principal shell (n)	Subshells	Orbitals	Electrons(e-)
1	1s	1	2
2	2s, 2p	1 + 3 = 4	2 + 6 = 8
3	3s, 3p ,3d	1 + 3 + 5 = 9	2 + 6 + 10 = 18
n ≥ 4	4s, 4p, 4d, 4f	1 + 3 + 5 + 7 = 16	2 + 6 + 10 + 14 = 32

Subshells

s — subshell
Orbitals :
Shape; spherical
Number: 1 (2e⁻)
s — Block:
Elements: group 1,2 ,H and He
Why?: Their highest energy electron is in the s subshell

p — subshell
Orbitals :
Shape: dumbbell
Number: 3 (6e⁻)
p — Block:
Elements: group 3—8
Why?: Their highest energy electron is in the p subshell

s orbital   p orbitals

2—Short hand
Rules:
1—strat with subshell that has the least energy
2—Replace the inner electrons that match a noble gas configuration with the symbol of that noble gas in brackets

Example:
Na(Z= 11):
Full: $1s^2\ 2s^2\ 2p^6\ 3s^1$
Nearest noble gas before Na: Neon (Ne) — $1s^2\ 2s^2\ 2p^6$
Shorthand: [Ne] $3s^1$

d — subshell
Orbitals :
Number: 5 (10e⁻)
f—block:
Elements: between groups 2,3

Why?: Their highest energy electron is in the d subshell
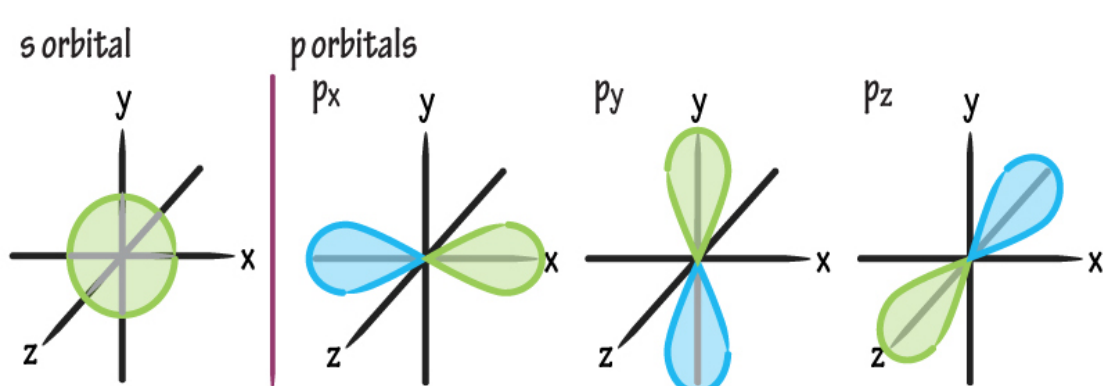
f — subshell
Orbitals :
Number: 7 (14e⁻)
f—block:
Elements: lanthanides and actinides
Why?: Their highest energy electron is in the f subshell

S P D F Blocks

Electronic configuration of atoms

1—Box form
Rules:
1—strat with subshell that has the least energy
2—e⁻ will occupy the orbital singly pefore pairing takes place
3—e⁻ in same orbital has opposite spins before pairing takes place

Examples:

Carbon (Z = 6):

Neon (Z = 10):

Cr (Z = 24):

observation: for Cu,Cr and element in thier groups the 4s orbital had only 1e

reason: these element would rather have only 1e in 4s to achive a half filled(d⁵) or filled subshell(d¹⁰) which is more stablw

observation: 4s was filled before 3d

reason: the 3d orbital has more energy than 4s (and like we said subshells are filled according to energy strating by least)

Cu (Z = 29):

3— Full configuration

Rules:

1—strat with subshell that has the least energy (1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p.)

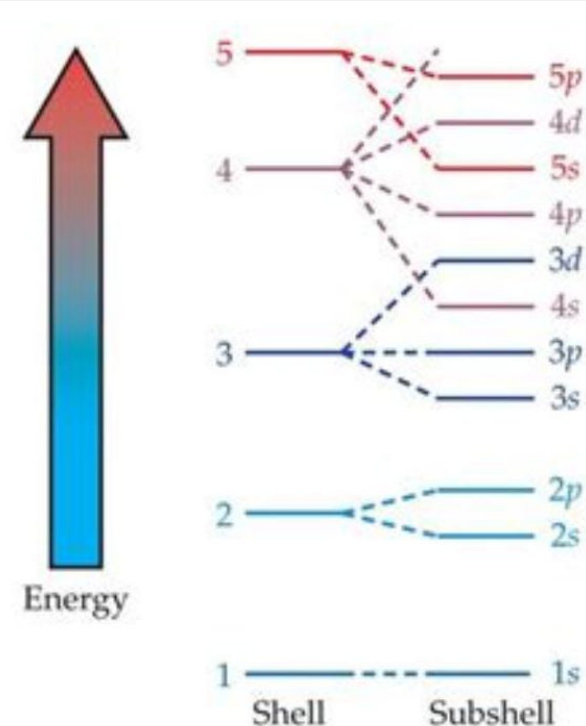| #	Element	Symbol	Electronic Configuration
1	Hydrogen	H	$1s^1$
2	Helium	He	$1s^2$
3	Lithium	Li	$1s^2 2s^1$
4	Beryllium	Be	$1s^2 2s^2$
5	Boron	B	$1s^2 2s^2 2p^1$
6	Carbon	C	$1s^2 2s^2 2p^2$
7	Nitrogen	N	$1s^2 2s^2 2p^3$
8	Oxygen	O	$1s^2 2s^2 2p^4$
9	Fluorine	Fl	$1s^2 2s^2 2p^5$
10	Neon	Ne	$1s^2 2s^2 2p^6$
11	Sodium	Na	$1s^2 2s^2 2p^6 3s^1$
12	Magnesium	Mg	$1s^2 2s^2 2p^6 3s^2$
13	Aluminium	Al	$1s^2 2s^2 2p^6 3s^2 3p^1$
14	Silicon	Si	$1s^2 2s^2 2p^6 3s^2 3p^2$
15	Phosphorous	P	$1s^2 2s^2 2p^6 3s^2 3p^3$
16	Sulphur	S	$1s^2 2s^2 2p^6 3s^2 3p^4$
17	Chlorine	Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$
18	Argon	Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$
19	Potassium	K	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
20	Calcium	Ca	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
21	Scandium	Sc	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$
22	Titanium	Ti	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$
23	Vanadium	V	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$
24	Chromium*	Cr	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$
25	Manganese	Mn	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^5$
26	Iron	Fe	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$
27	Cobalt	Co	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^7$
28	Nickel	Ni	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$
29	Copper*	Cu	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$
30	Zinc	Zn	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$
31	Gallium	Ga	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^1$
32	Germanium	Ge	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^2$
33	Arsenic	As	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^3$
34	Selenium	Se	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^4$
35	Bromine	Br	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$
36	Krypton	Kr	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$

observation: 4s was filled before 3d

reason: the 3d orbital has more energy than 4s (and like we said subshells are filled according to energy strating by smallest)

Electronic configuration of ions

Rules:

1—remove the e⁻ from the obital with highest energy

2—the electron are removed from 4s before 3d

Atomic radius

Down a group: the atomic radius increases:

　Addition of a New Shell: Each element adds a new principal energy level (e.g., n=2 to n=3), placing the valence electrons farther from the nucleus.

　Increased Shielding: The inner core of electrons shields the valence electrons from the full attractive force of the nucleus.

　Increased Energy/repuslion: More electrons in the outer shell lead to greater electron—electron repulsion, which pushes the electron cloud outward.

　Weaker Effective Nuclear Pull: The combined effect of greater distance and stronger shielding means the valence electrons experience a weaker force(eventhough the nuclear charge increases).

Across a period (left to right), the atomic radius decreases.

　Increasing Nuclear Charge: The number of protons in the nucleus increases with each element.

　Constant Shielding: Electrons are added to the same principal energy level, so the shielding by inner electrons remains constant.

　Stronger Effective Nuclear Pull: The increasing nuclear charge pulls the electron cloud closer to the nucleus without being counteracted by additional shielding.

　More tightly held
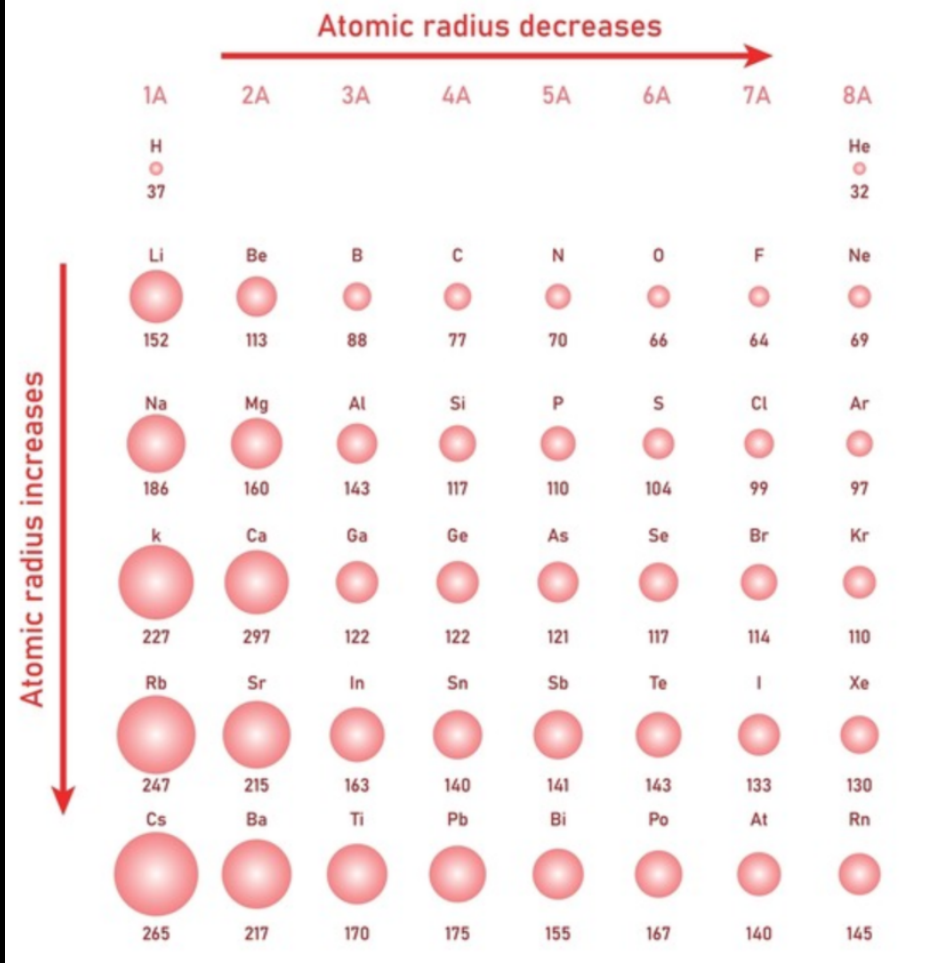
Ionic radius

Cations are always smaller than their parent atoms.

　Loss of an Electron Shell: When a cation forms, the entire outer valence shell of electrons is often lost.

　Increased Proton—to—Electron Ratio: The atom loses electrons but retains the same number of protons, leading to a greater nuclear charge per remaining electron.

　Reduced Electron Repulsion: Fewer electrons mean less electron—electron repulsion, allowing the electron cloud to be pulled inward.

　More tightly held
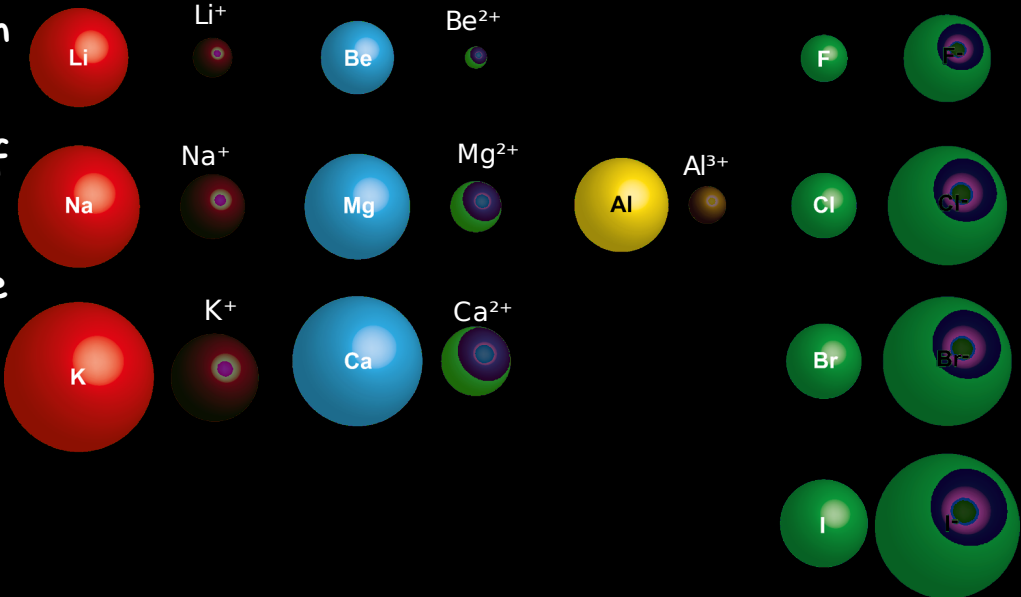
Anions are always larger than their parent atoms.

　Gain of Electrons: The atom gains extra electrons into its existing valence shell.

　Decreased Proton—to—Electron Ratio: The nuclear charge remains the same, but it is now spread over a larger number of electrons, reducing the nuclear charge per electron

　Increased Electron Repulsion: The additional electrons increase the repulsive forces within the electron cloud, pushing electrons further apart.

　less tightly held

Ionization energy

Ionisation energy (IE): The amount of energy needed to remove one mole of electrons from one mole of gaseous atoms.(endothermmic)

　1st Ionization Energy (IE_1): The amount of energy needed to remove one mole of the most loosely held electrons from one mole of gaseous atoms to form one mole of +1 gaseous cations.

　　General Equation: $X(g) \rightarrow X^+(g) + e^-$
　　Examplex: $Na(g) \rightarrow Na^+(g) + e^-$

　2nd Ionization Energy (IE_2): The amount of energy needed to remove one mole of electrons from one mole of +1 gaseous cations to form one mole of +2 gaseous cations.

　　General Equation: $X^+(g) \rightarrow X^{2+}(g) + e^-$
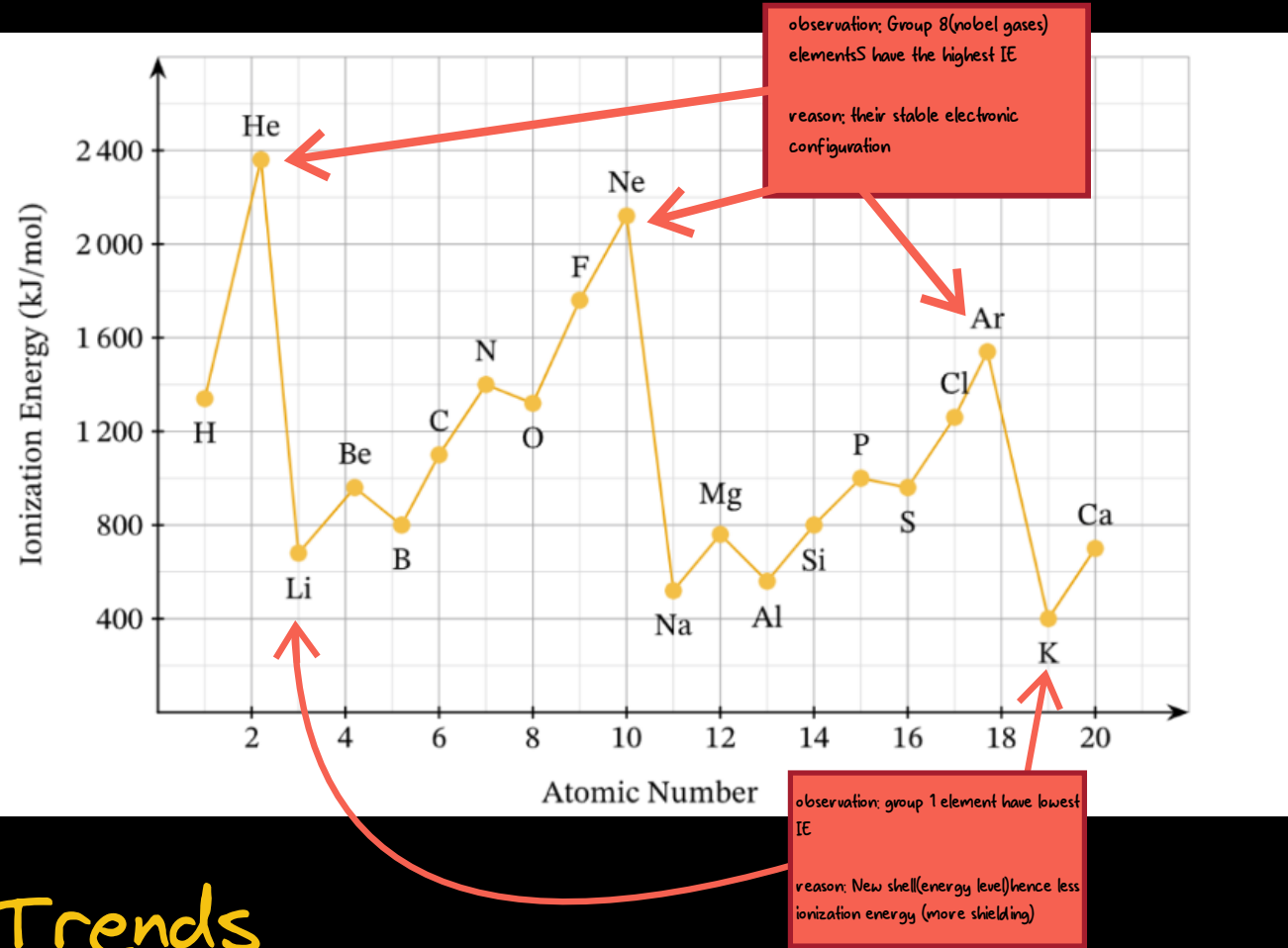　　Example: $Na^+(g) \rightarrow Na^{2+}(g) + e^-$

　3rd Ionization Energy (IE_3): The amount of energy needed to remove one mole of electrons from one mole of +2 gaseous cations to form one mole of +3 gaseous cations.

　　General Equation: $X^{2+}(g) \rightarrow X^{3+}(g) + e^-$
　　Example: $Mg^{2+}(g) \rightarrow Mg^{3+}(g) + e^-$

Your Notes

Ionization energy

observation: Group 8(nobel gases) elementS have the highest IE

reason: their stable electronic configuration

observation: group 1 element have lowest IE

reason: New shell(energy level)hence less ionization energy (more shielding)

Trends

IE Increases Across a Period
   Higher nuclear charge (more protons)
   Smaller atomic radius (same shell)
   Stronger attraction to the nucleus (increased effective nuclear charge)
   Shielding is constant (no new inner shells)

IE Decreases Down a Group
   New electron shell added (outer electrons are farther away)
   Increased Energy (level)
   Increased shielding from inner electrons (electron-electron repuslion)
   Larger atomic radius (weaker nuclear attraction)
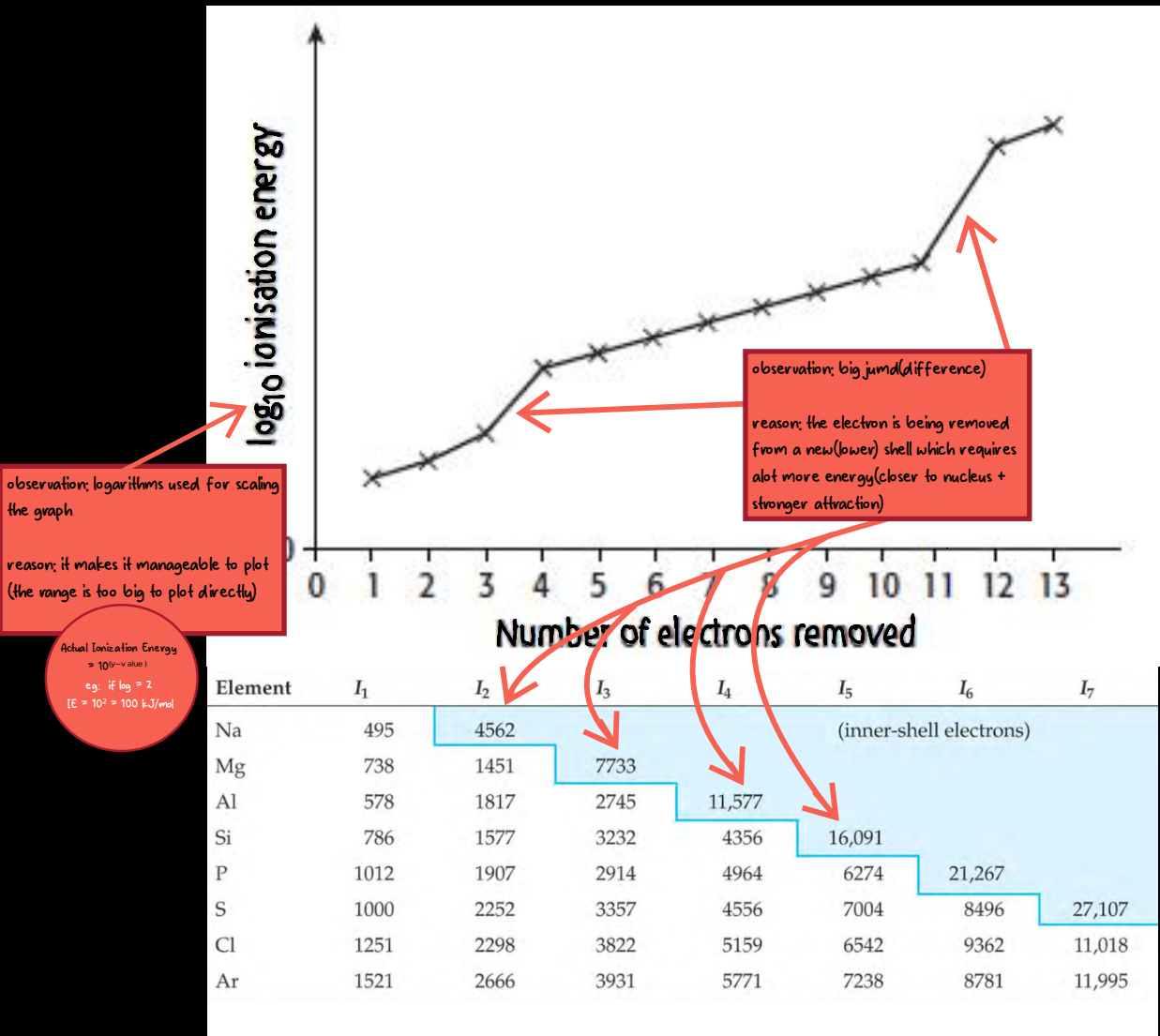   Result: The nuclear pull on the outermost electron weakens.

Exception: Boron < Beryllium (Al < Mg)
   B: Electron removed from a higher energy 2p orbital.
   Be: Electron removed from a stable, lower energy 2s orbital.
   The 2p electron is also shielded by the 2s subshell and on a higher
energy evel, making it easier to remove.

Exception: Oxygen < Nitrogen (S < P)
   both: Removed from p shell
   O: Electron removed from a paired 2p orbital.
   N: Electron removed from a stable, half-filled 2p subshell.
   Spin-pair repulsion in the paired orbital makes the electron easier to
remove(reduces ionization energy).

Your Notes

Successive ionization energies

observation: logarithms used for scaling the graph

reason: it makes it manageable to plot (the range is too big to plot directly)

Actual Ionisation Energy
= $10^{(x-axis)}$
e.g. if log = 2
IE = 10^2 = 100 kJ/mol

observation: big jump(difference)

reason: the electron is being removed from a new(lower) shell which requires alot more energy(closer to nucleus + stronger attraction)

Element	I_1	I_2	I_3	I_4	I_5	I_6	I_7
Na	495	4562			(inner-shell electrons)		
Mg	738	1451	7733				
Al	578	1817	2745	11,577			
Si	786	1577	3232	4356	16,091		
P	1012	1907	2914	4964	6274	21,267	
S	1000	2252	3357	4556	7004	8496	27,107
Cl	1251	2298	3822	5159	6542	9362	11,018
Ar	1521	2666	3931	5771	7238	8781	11,995

There would be a general increase
1-electron (lesss repulsion
2-radius decreases
3-ion becomes more positive

Melting and boiling points
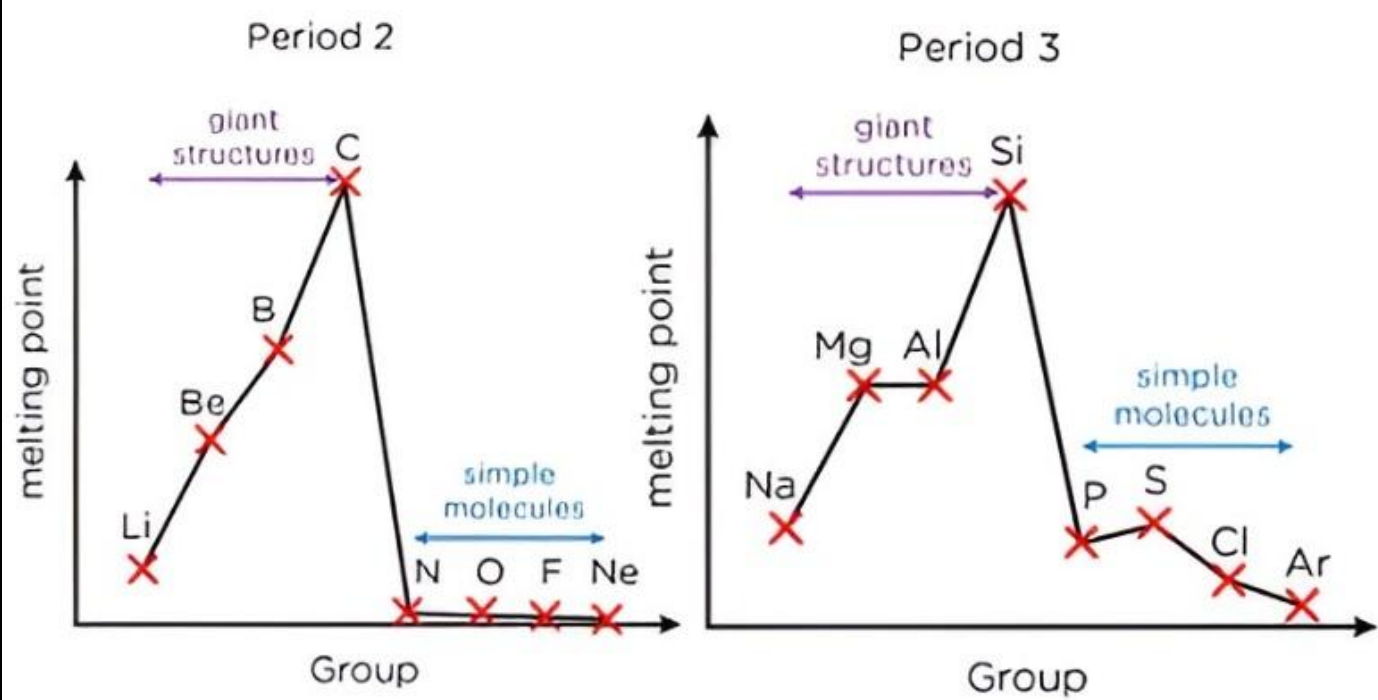
Period 2	Li	Be	B	C	N	O	F
M.P/B.P	High	High	High	High	Low	Low	Low
Conductivity	good	good	bad	bad	bad	bad	bad
bonding type	Metalic	Metalic	Covelant	Covelant	Covelant	Covelant	Covelant
structure	Giant	Giant	Giant	Giant	simple molecular	simple molecular	simple molecular

Period 3	Na	Mg	Al	Si	P	S	Cl
M.P/B.P	High	High	High	High	Low	Low	Low
Conductivity	good	good	good	bad	bad	bad	bad
bonding type	Metalic	Metalic	Metalic	Covelant	Covelant	Covelant	Covelant
structure	Giant	Giant	Giant	Giant	simple molecular	simple molecular	simple molecular

Across period
Na-Al(Li-Be):
1-melting/boiling points: increase as there are strong metallic bond that get stronger(harder to overcome) with more delocalized electron
2-Conductivity: Good and increases as there are more delocalized electron

Si(B-C):
1-Melting/boiling points: high (highest at C/Si) as they are held by strong covelant bonds forming a Giant structure (requires alot of energy to overcome forces)
2-Conductivity: bad as there are no free electrons

P-Cl(N-F):
1-Melting/boiling points: low (lowest at Cl/F) as molecules are held by weak forces(london force) forming a simple molecular structure that are easy and require little energy to overcomeAmong the common molecular elements in Period
Notes: Among (P_4, S_8, Cl_2), Sulfur (S_8) has the strongest intermolecular forces due to its larger molecule.
2-Conductivity: bad as there are no free electrons